Reynolds' Transport Theorem in a Discrete System

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Outline

Introduction

- Reynolds' transport theorem
- Discrete models (molecular dynamics)
- Irving and Kirkwood (1950)
- . Discrete Form of Reynolds' Transport Theorem
 - Control Volume Function
 - Reynolds' transport theorem using the control volume function
 - Application to microscopic pressure
- . Results
 - Numerical simulations of Couette flow and shockwaves
 - Applying the method to coupling
 - Application to other discrete systems

Introduction



Reynolds' Transport Theorem

- Conversion of a Lagrangian system to an Eulerian Control
 Volume
 - Mass Conservation

$$\begin{aligned} \frac{d}{dt} \int_{V} \rho dV &= 0 \\ &= \int_{V} \frac{d\rho}{dt} dV + \oint_{S} \rho \boldsymbol{u} \cdot d\boldsymbol{S} \end{aligned}$$

Momentum Balance

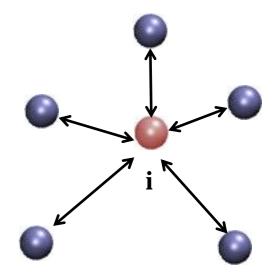
$$\begin{split} \frac{d}{dt} \int_{V} \rho \boldsymbol{u} dV - F_{surface} &= 0 \\ &= \int_{V} \frac{d\rho \boldsymbol{u}}{dt} dV + \oint_{S} \end{split}$$

$$\oint \rho u u \cdot dS - F_{surface}$$

Discrete models (molecular dynamics)

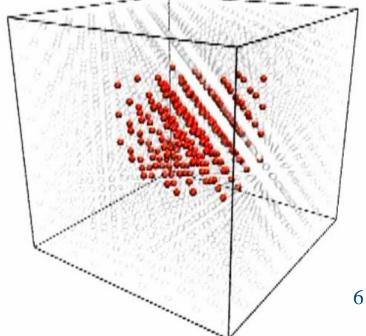
- . Discrete Molecules in continuous space
 - . Governed by Newton's Law for an N-body system
 - Point particles with pairwise interactions only

$$m_i \ddot{\boldsymbol{r}}_i = \mathbf{F}_i = \sum_{i \neq j}^N \boldsymbol{f}_{ij} \qquad egin{array}{cc} \ddot{\boldsymbol{r}}_i
ightarrow \dot{\boldsymbol{r}}_i \ \dot{\boldsymbol{r}}_i
ightarrow m{r}_i(t) \end{array}$$



- Discrete N-body system defined in terms of sums
 - Sum over entire system defines Lagrangian system
 - How do we get an Eulerian description?

$$\rho_{system} = \frac{1}{M} \sum_{i=1}^{M} m_i \qquad \int_{V} \rho(\boldsymbol{r}, t) dV = ?$$



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(2.3) for the probability distribution in Gross phase space and then perious repealed laterations. Since * This work was supported by the U.S. ONR under Oxtract Ninatr 244 with the California Indirect of Twelmenby, J. G. Kirkwood, J. Chem. Phys. 14, 30 (1046)

derived. If so doing, the stress tensor and boll current density can be expressed in terms of molecular variables. The stress service consists of a location of the location uncar in gramerus of thud velocity and, 'herely', ec-pressiona (in terms of enderular variables) (ar co-efficients of abear and volume viscosity.) The same density can be expressed in terms of molecular variables. The stress tensor consists of a kinetic part (which exerts in the kinetic stress of a kinetic part (which (dominant for a liquid) which will be expressed as a moderature involving the constraint of intermetation trommant for a neural which will be expressed as a quadrature involving the potential of intermulecular force and the sensity of extential of endowine or in know quadrature involving the potential of intermalecular force and the tensity of pairs of molecules. The hert nore and the versity of pairs or molecules. The best surrent density is the sum of the isrniliar kinetic part current density is the arm of the forminar unger par-and a quarketure involving the potential of inter-noicentar force and the density and current density and the content of the density and current density and the content of the density of currents are the second noncenar torce and the density and current density in the configuration space of a pair of molecular. The re-oble some resolution states in the fact reside of some the contiguration space of a pair of non-enders. The re-sults were previously stated in the first article of this arties, when this definition was promised. To obtain explicit expressions for the pair probability density and revealability expressions denotes are sensed to To obtain explicit expressions for the pair probability density and probability current density one would in principle need to police the Linuville equation [Eq. (2.3)] for the grobability distribution in Gives phase over fact, then readous constant terministic Since

approximately by the probability distribution function in the phase space of a rair of molecules, One such repair tion has been derived by Born and Greene using a generalized "superposition" assumption. Another, a THIS paper will be concerned with a derivation of the equations of hydrodynamics from the min reacting aperiositica assumption. Another, generalization of the well-known Fokker-Planck equigeneralization of the well-known rocker-rance coun-tion of stochastic theory, has been derived by Kjrkthe equations of hydrodynamics including the policities of the classical statistical mechanics. In parciples of the classical statistical mechanics, in par-ticular, the equation of continuity, the equador of mening, and the equation of energy transport will be notion, and the equation of energy transport will be derived. By so doing, the stress tensor and heat current derived and be an energy to be a

The equations of hydrolynamics—conticulty equation, equation of easier, and repeaters un obtained tradpert- are derive with beam of the classic contribution mechanics. Thereby, oppeations us the familiar for the system tensor with beam of the classic contribution of another analysis. In addition, the familiar for the system tensor is a structure of easier in terms of understand yours intermediate terms. The terms of the system tensor is a structure of the system terms of understand and the system of the system case beam of the system of the system terms of understand and the system of the system convolutions of intermedication to the threat terms of understand and an enderstand as quadratures of the density and currents, density in the configuration space of a pair of understand as quadratures of the density and currents. this program is untenable for a liquid, various attempts uns program se untenance nor a injun, vanous autorigas have been made to obtain a closed equation satisfied have been made to obtain a closed equation satisfied have been made to obtain a closed equation satisfied approximately by the probability distribution function

The Statistical Mechanical Theory of Transport Processes. IV. The Equations of Hydrodynamics* THE INCREAT OF CREMICAL PHYSICS J. H. Invited AND JUNE G. EUROWOOD Gates and Crelline Jahrmieries of Chemistry No. 1343, Passdene, California (Resoluted Konsender 31, 1963).

88 3X 395, the rather large difference between calculated and observed frequency being ascribed to the proximity and observed incruency being ascriber, to its proximity to the A, fundamental. However, this hand could be an to the A_2 inneamental. However, this band could be an upper-stage band corresponding to S19 cm⁻¹. The interpretation of the faint sharp lund at 769.4 cm⁻¹ as an upper-stage band, 778 + ν_{-2} scenar more abundle then its interpretation on the R_{-1} and R_{-2} cm⁻⁻ as an upper-stage band, $778+e_1-e_0$ scents more plausible than its interpretation as the B_{10} combinition 3101-552 cm⁻¹. The first show become band as each plausible than its interpretation as the H w combinement. 2104-558 cm⁻¹. The faint sharp Raman band at \$28.5 lata in the long wave-kngth region. 210+558 cm⁻¹. The faint sharp Raman band at 835. cm⁻¹ has been interpreted as an upper-stage band. 2X a07+ve−ve, rabter than as the B₂, difference band 1540-510 cm⁻¹, because the corresponding cam band VULUME 15. NUMBER 6

171.9 cm⁻¹. The band at 809.7 cm⁻¹ has been interpreted 17: 9 cm⁻⁴. The band at 309.7 cm⁻¹ has been interpreted as 22×394, the rather large difference between calculated and decoursed forements being standard to the recommend The writers wish to express their inceptedness to Dr. The writers wan to express their incediedness to Dr. C. F. Hanmer and E. L cn Pont de Nemours and C. F. Hammiter and E. L Gu Pont de Nemours and Company for the samples; to Doctors Isabella and Jerome Karle for electron differential data; and to Dr. V. Buden et due Matteret Bused at Secondari Leve Jerome Karle lor electron diffraction dats; and in Dr. E. K. Phyler and the National Bureau of Standards for

has not been observed. If the preferred interpretations TRANSPORT PROCESSES this hot been ouserved, it the preferren interpretations are correct, the group of Raman hands, 769, 778, 819, and 829 cm², are related to each other in much the same and 8.5% cm⁻¹, are related to each other in much the same manner as similar groups in the spectra of CO₂ and CS₂.

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M. Boss and M. S. Creen. Proc. Roy. Soc. ABS 10 (1996). N. Boss and M. S. Creen. Proc. Roy. Soc. ABS 10 (1996). N. Edwards, Burdy and Taren, J. Chem. Proc. Article and the social strain and the s

Irving and Kirkwood (1950)

511-10 $S(x_n) f(x,v) du = f(v,v)?$ The probability distribution function (relative den-as the expectation value of the dynamical variable sity of representative points in phase space) we denote $d' \int F s = \frac{1}{2} \int f s = \frac$ satisfying the normalize tion condition $\int \cdots \int f d\mathbf{R}_{t} \cdots d\mathbf{R}_{t} d\mathbf{p}_{t} \cdots d\mathbf{p}_{t'} = 1$ where $d\mathbf{R}_{4}$ stands for a volume element in the con-Ware det stands for a volume exement in the con-figuration space and de à volume element in the con-menture answer of the still review the schemas in time. (2.1) Eguration space and dp, a volume element in the mo-mentany space of the 4th moderate f charges in time accounting on the well-become time the equation mentum space of the till molecule. ' changes according to the well-known Liouville equation 102 $\frac{df}{dt} = \sum_{k=0}^{N} \left[-\frac{p_k}{m_k} \nabla R_k f + \nabla R_k U \cdot \nabla p_k f \right]$

 $\langle a_i f \rangle = \int \dots \int a \langle \mathbf{R}_{l_1} \dots \mathbf{p}_{l_{i-1}} \rangle f (\mathbf{R}_{l_1} \dots \mathbf{p}_{l_{i-1}}) f (\mathbf{R}_{l_1} \dots \mathbf{p}_{l_{i-1}}, l)$

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+ (a; Ve, U. Vou!)]. (2.4)

 $\frac{\partial}{\partial t}(\alpha_i, f) = \left(\alpha_i, \frac{\partial f}{\partial t}\right) = \sum_{k=1}^{N} \left[\left(\alpha_i, \frac{\mathbf{P}_k}{\mathbf{m}_k}, \frac{\mathbf{P}_k}{\mathbf{m}_k}\right) \right]$

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Thus, (2.4) becomes

By Green's theorem applied in the space of R.

providing the integrated part vanishts; i.e., providing the gyalem is bounded or falls of sufficiently rapid as R and Likewise, since Tack' is independent of rapid

the gystem x bounded or f tails of sufficiently tags as $R_{k} \rightarrow \infty$. Likewise, since $\nabla R_k f$ is independent of mentum n, and since f is in or satisfies an interval

is $K_{k} \to \infty$. Likewise, since V_{k+1} is unependent meature p_{k} and since f falls off rapidly is p_{k-1}

of Green's theorem in the momentum space of g

(a; VR& U. Vp. f) = - (VR&U. Vp. a; f

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Sol PA VERCE VEGU: VEGUE, We shall use (2.7) to derive the equations of hydro- Avnomize

III. STATISTICAL MECHANICAL EXPRESSIONS FOR DENSITIES The equations of hydrodynamics (1.1), (1.2), and (1.4) are concerned with densities in ecdancy 3-space, e.g., mass density, momentum density, and energy density. We shall now express these as the expectation values of hydramical variables over an ensemble baving distribution function f.

81 $\int \delta(\mathbf{R}_{0}-\mathbf{r})f(\mathbf{R}_{d_{1}},\cdots,\mathbf{p}_{t_{1}},\cdots,\mathbf{t})d\mathbf{R}_{t}\cdots d\mathbf{p}_{t_{N}}$ pro (Re + Solt) apple and I look Eldright - mx prints. The lotal that & density at r due to all audocules is thus

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 $(p_1, \dots, p_i, \dots, p_i)$ where the integration is over all position vectors are all p_1, \dots, p_i where the integration is over all position vectors are all position vecto

others are a

where C is the potential energy of the entire system. Any cynamical variable, $\alpha(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{R}_1, \dots, \mathbf{R}_N)$, bas an expectation value given at time f by

 $P(z; t) - \sum_{k=1}^{N} m_k (\delta(\mathbf{R}_k - \mathbf{r}));$

 $\int \rho_{i\delta}(\mathbf{R}_{i}-r)/(\mathbf{R}_{i_{1}}\cdots;\rho_{i}\cdots;i)d\mathbf{R}_{i_{1}}\cdots d\rho_{i_{\ell}}$

id the locations of the

 $\int \cdots \int \delta(\mathbf{R}_{i} - \mathbf{r}) f(\mathbf{R}_{i_{1}} \cdots ; \mathbf{p}_{i_{1}} \cdots ; i) d\mathbf{R}_{1} \cdots d\mathbf{p}_{n},$

at the eth molecule to the momentum per unit values (mass current decas(y). The local momentum decasity

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it is at

(2.5)

 $\rho(\mathbf{r},t) = \sum m_i \delta\left(\mathbf{r} - \mathbf{r}_i\right)$

 $\int \cdots \int f(\mathbf{R}_1, \cdots, \mathbf{p}_l, \cdots, i) d\mathbf{R}_1 \cdots$

instribution function f. The probability per unit volume that the $\pm th$ molecules be as $R_{\rm e}$ is

Selecting Functions

The Dirac delta selects molecules at a point

- Infinitely high, infinitely thin peak •
- Equivalent to the continuum differential • formulation at a point

$$\rho(\boldsymbol{r},t) = \sum_{i=1}^{N} m_i \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right)$$

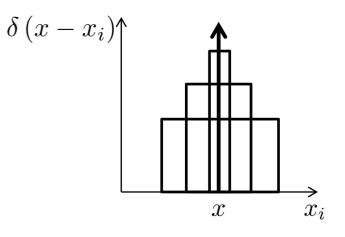
Cannot be applied directly in a molecular • simulation as r_i is never exactly equal to r

Relaxed weighting function used by • Hardy(1981), Hoover (2009), Murdoch (2010) and others

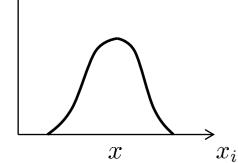
$$\rho(\mathbf{r},t) \neq \sum_{i=1}^{N} m_i \Delta \left(\mathbf{r} - \mathbf{r}_i\right)$$

$$(\boldsymbol{r},t) \neq \sum_{i=1}^{N} m_i \Delta (\boldsymbol{r} - \boldsymbol{r}_i)$$

$$\Delta \left(x - x_i \right)^{\uparrow}$$







Discrete Reynolds' Transport Theorem



More information

• Further details of mathematics and numerical simulations are available in the recently published paper in Physical Review E

PHYSICAL REVIEW E 85, 056705 (2012)

Control-volume representation of molecular dynamics

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Department of Mechanical Engineering, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom (Received 13 October 2011; revised manuscript received 2 March 2012; published 22 May 2012)

A molecular dynamics (MD) parallel to the control volume (CV) formulation of fluid mechanics is developed by integrating the formulas of Irving and Kirkwood [J. Chem. Phys. 18, 817 (1950)] over a finite cubic volume of molecular dimensions. The Lagrangian molecular system is expressed in terms of an Eulerian CV, which yields an equivalent to Reynolds' transport theorem for the discrete system. This approach casts the dynamics of the molecular system into a form that can be readily compared to the continuum equations. The MD equations of motion are reinterpreted in terms of a Lagrangian-to-control-volume (\mathcal{LCV}) conversion function ϑ_i for each molecule *i*. The \mathcal{LCV} function and its spatial derivatives are used to express fluxes and relevant forces across the control surfaces. The relationship between the local pressures computed using the volume average [Lutsko, J. Appl. Phys. 64, 1152 (1988)] techniques and the method of planes [Todd *et al.*, Phys. Rev. E 52, 1627 (1995)] emerges naturally from the treatment. Numerical experiments using the MD CV method are reported for equilibrium and nonequilibrium (start-up Couette flow) model liquids, which demonstrate the advantages of the formulation. The CV formulation of the MD is shown to be exactly conservative and is, therefore, ideally suited to obtain macroscopic properties from a discrete system.

DOI: 10.1103/PhysRevE.85.056705

PACS number(s): 05.20.-y, 47.11.Mn, 31.15.xv



Control Volume Function

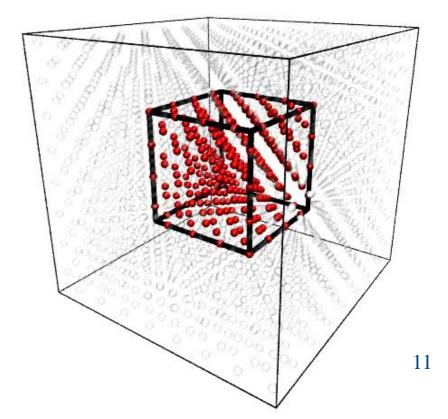
• The Control Volume function is the integral of the Dirac delta function in 3 Dimensions

$$\vartheta_i \equiv \int_{x^-}^{x^+} \int_{y^-}^{y^+} \int_{z^-}^{z^+} \delta(x_i - x) \delta(y_i - y) \delta(z_i - z) dx dy dz$$

$$= [H(x^{+} - x_{i}) - H(x^{-} - x_{i})]$$

$$\times [H(y^{+} - y_{i}) - H(y^{-} - y_{i})]$$

$$\times [H(z^{+} - z_{i}) - H(z^{-} - z_{i})]$$



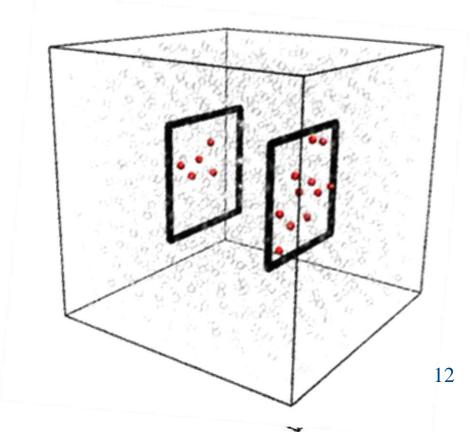
Derivatives yields the surface flux

. Taking the Derivative of the CV function

$$dS_{ix} \equiv -\frac{\partial \vartheta_i}{\partial x_i} = \left[\delta(x^+ - x_i) - \delta(x^- - x_i)\right] \\ \times \left[H(y^+ - y_i) - H(y^- - y_i)\right] \\ \times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$

• Surface fluxes over the top and bottom surface

$$dS_{ix} = dS_{ix}^+ - dS_{ix}^-$$



Applying the Control Volume Function

. Molecular mass in a control volume can be defined

$$\frac{d}{dt} \int_{V} \rho d(\mathbf{V}, t) = \frac{d}{dt} \sum_{i=1}^{N} m_{i} \vartheta(\mathbf{r} - \mathbf{r}_{i})$$

• Simple mathematical operations using the control volume function

$$\frac{d}{dt} \sum_{i=1}^{N} m_i \vartheta_i = \sum_{i=1}^{N} \left(\vartheta_i \frac{d}{dt} / m_i + m_i \frac{d}{dt} \vartheta_i \right)$$
$$= \sum_{i=1}^{N} m_i \frac{d\mathbf{r_i}}{dt} \cdot \frac{d}{d\mathbf{r_i}} \vartheta_i$$
$$= -\sum_{i=1}^{N} m_i \mathbf{v}_i \cdot d\mathbf{S}_i$$
College

Reynolds' Transport Theorem

- Mass, momentum and energy equations
 - Mass Conservation

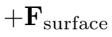
$$\frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \cdot d\mathbf{S}_i$$

$$\frac{\partial}{\partial t} \int_{V} \rho dV = -\oint_{S} \rho \boldsymbol{u} \cdot d\mathbf{S}$$

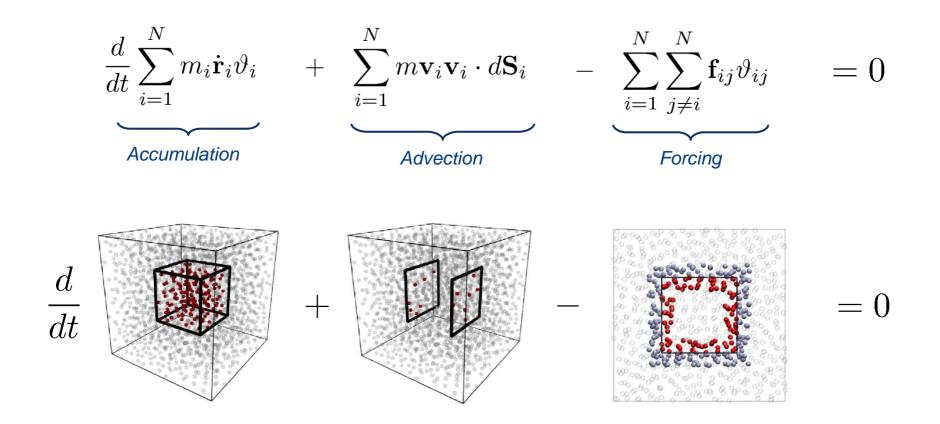
Momentum Balance

$$\frac{d}{dt} \sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i + \sum_{i=1}^{N} \sum_{j \neq i}^{N} \mathbf{f}_{ij} \vartheta_{ij}$$

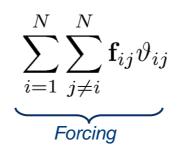
$$\frac{\partial}{\partial t} \int_{V} \rho \boldsymbol{u} dV = -\oint_{S} \rho \boldsymbol{u} \boldsymbol{u} \cdot d\mathbf{S}$$

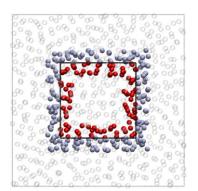


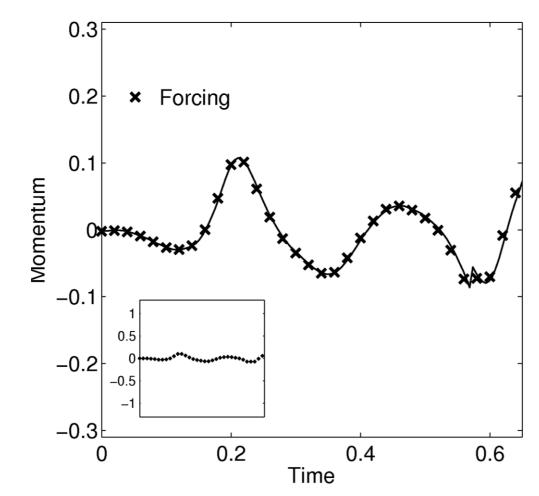
. Momentum Balance



. Momentum Balance



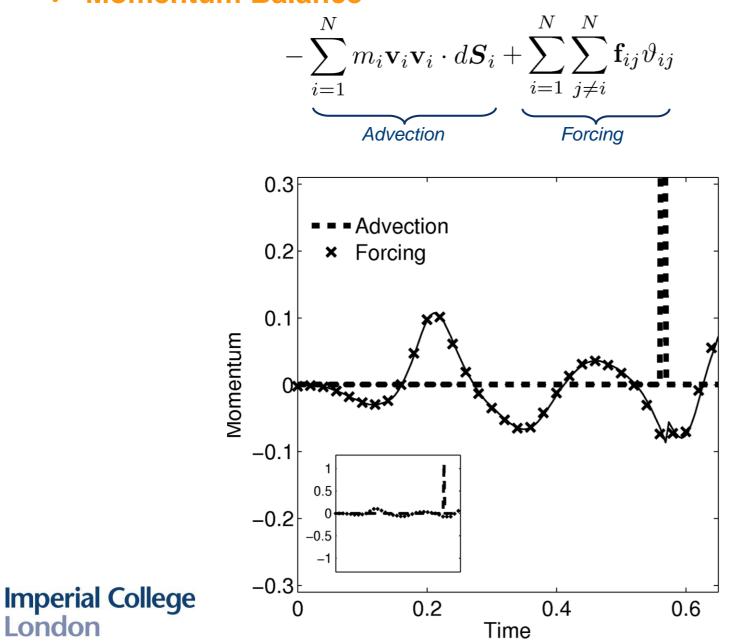


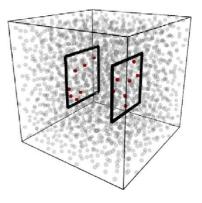


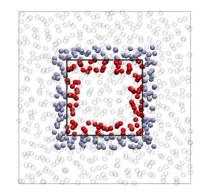
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Momentum Balance

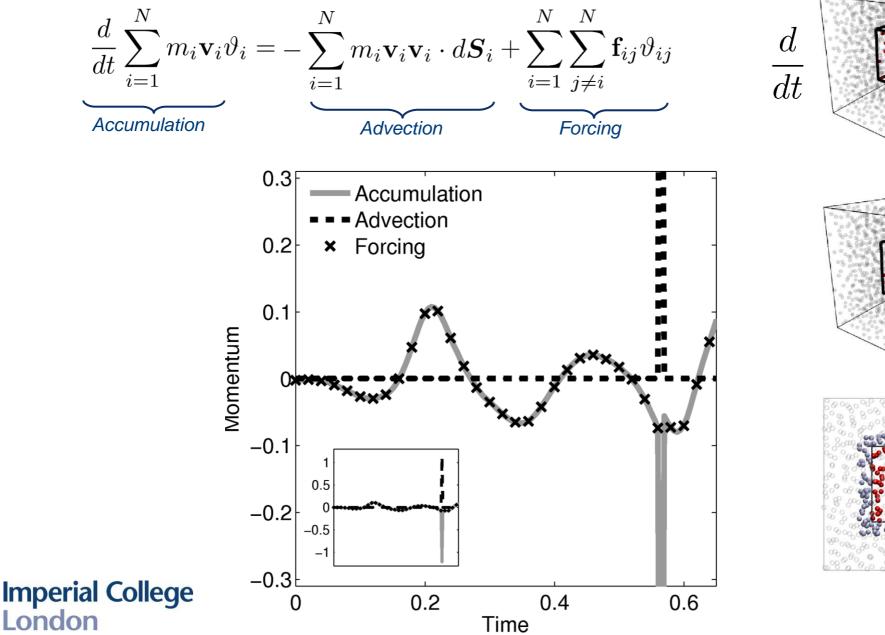
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. Momentum Balance

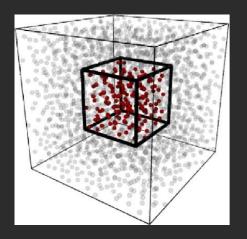


Divergence of Pressure

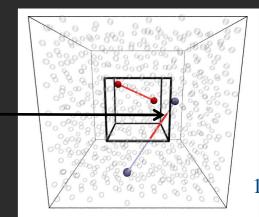
- . The momentum balance equation can be re-written in terms of the divergence of pressure
 - Momentum Balance

$$\begin{split} \frac{d}{dt} \sum_{i=1}^{N} m_{i} \mathbf{v}_{i} \vartheta_{i} &= -\int_{V_{i}}^{N} \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{u} \mathbf{u} d\mathbf{S}_{i} & \frac{\partial}{\partial t} \int_{V} \rho \mathbf{u} dV = -\oint_{V_{i}} \frac{\partial}{\partial \mathbf{r}} \rho \mathbf{u} d\mathbf{S}_{i} \\ -\frac{\partial}{\partial \mathbf{r}} \cdot \sum_{i=1}^{N} \left[\left(\mathbf{v}_{i} - +\sum_{i=1}^{N} \sum_{j \neq i}^{N} \mathbf{f}_{ij} \vartheta_{ij} + \sum_{j \neq i}^{N} \mathbf{f}_{ij} \mathbf{r}_{ij} \int_{0}^{1} \vartheta_{s} ds \right] & - + \int_{V} \frac{\partial}{\partial \mathbf{r}} \mathbf{r} \partial \mathbf{r} dV \\ - \int_{V} \frac{\partial}{\partial \mathbf{r}} \mathbf{r} \partial \mathbf{r} \partial \mathbf{r} dV = -\int_{V} \frac{\partial}{\partial \mathbf{r}} \mathbf{r} \partial \mathbf$$

Volume Average Form of Lutsko (1988) & Cormier et al (2001)



$$\vartheta_{ij} = \sum_{\alpha=1}^{3} \frac{\partial}{\partial r_{\alpha}} \int_{0}^{1} \vartheta_{s} ds -$$



Surface Pressures

- The momentum balance equation can be re-written in terms of pressure over the control volume surfaces
 - . Momentum Balance

. The derivative of ϑ_s is the forces acting over the surface a localisation of the method of planes (Todd et al 1995)

$$\vartheta_{ij} = \sum_{\alpha=1}^{3} \frac{\partial}{\partial r_{\alpha}} \int_{0}^{1} \vartheta_{s} ds = dS_{xij} + dS_{yij} + dS_{zij}$$

Results and Applications



у

Continuum Analytical

• Simplify the momentum balance (Navier-Stokes) equation

$$\frac{\partial}{\partial t}\boldsymbol{u} + \boldsymbol{\nabla} \cdot \boldsymbol{u} \boldsymbol{u} = \frac{1}{\rho} \boldsymbol{\nabla} \boldsymbol{P} + \frac{\mu}{\rho} \boldsymbol{\nabla}^2 \boldsymbol{u}$$

• Solve the 1D unsteady diffusion equation.

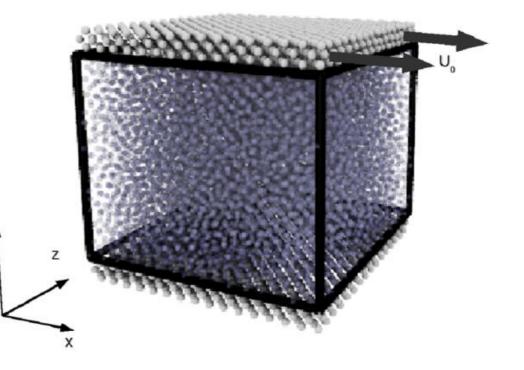
$$\frac{\partial u_x}{\partial t} = \frac{\mu}{\rho} \frac{\partial^2 u_x}{\partial y^2}$$

• With Boundary Conditions

$$u_x(0,t) = 0$$
$$u_x(L,t) = U_0$$
$$u_x(y,0) = 0$$

• Molecular Dynamics

• Fixed bottom wall, sliding top wall with both thermostatted



Continuum Analytical

• Simplify the control volume momentum balance equation

$$\frac{\partial}{\partial t} \int_{V} \rho \boldsymbol{u} dV = -\oint_{S} \rho \boldsymbol{u} \boldsymbol{u} \cdot d\boldsymbol{S}$$
$$-\oint_{S} P \boldsymbol{I} \cdot d\boldsymbol{S} + \oint_{S} \boldsymbol{\sigma} \cdot d\boldsymbol{S}$$

. Simplifies for a single control volume

$$\frac{\partial}{\partial t}\int_{V}\!\!\!\!\rho u_{x}dV\!=\!\int_{S_{y}^{+}}\!\!\!\!\!\sigma_{xy}dS_{f}^{+}\!-\!\int_{S_{f}^{-}}\!\!\!\!\!\!\sigma_{xy}dS_{y}^{-}$$

• With Boundary Conditions

$$u_x(0,t) = 0$$
$$u_x(L,t) = U_0$$
$$u_x(y,0) = 0$$

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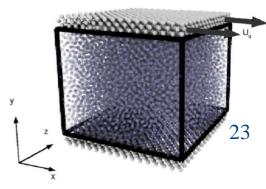
- Molecular Dynamics
 - Discrete form of the Momentum balance equation

$$\frac{d}{dt} \sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\oint_S \rho \boldsymbol{u} \boldsymbol{u} \cdot d\boldsymbol{S}$$
$$-\sum_{i=1}^{N} (\boldsymbol{v}_i - \boldsymbol{u}) (\boldsymbol{v}_i - \boldsymbol{u}) \cdot d\boldsymbol{S}_i - \sum_{i=1}^{N} \sum_{j \neq i}^{N} \varsigma_{ij} \cdot d\boldsymbol{S}_{ij}$$

• Simplifies for a single control volume

$$\frac{d}{dt}\sum_{i=1}^{N}m_i\mathbf{v}_i\vartheta_i = \sum_{i,j}^{N}f_{xij}dS_{yij}^+ - \sum_{i,j}^{N}f_{xij}dS_{yij}^-$$

• Fixed bottom wall, sliding top wall with both thermostatted

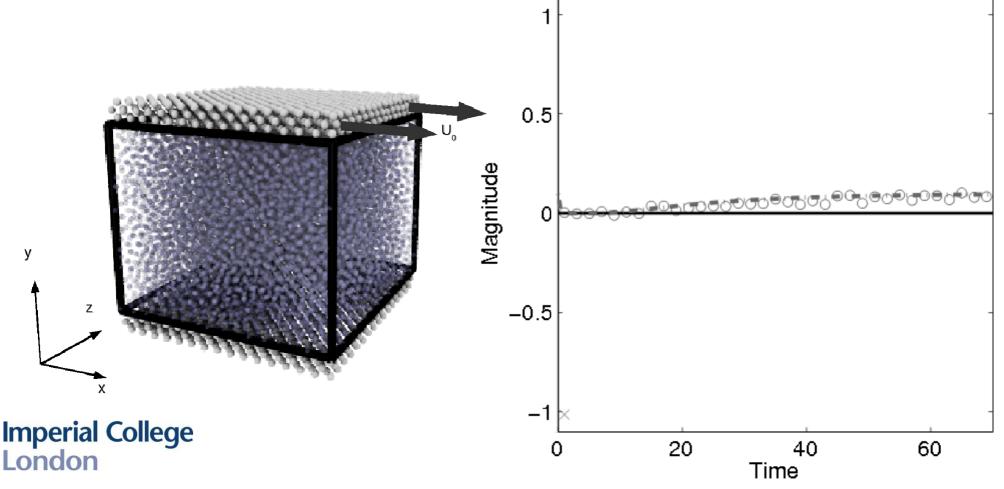


. Simulation setup

- Starting Couette flow
- Wall thermostat: Nosé-Hoover
- Averages are computed over 1000 time steps and 8 realizations

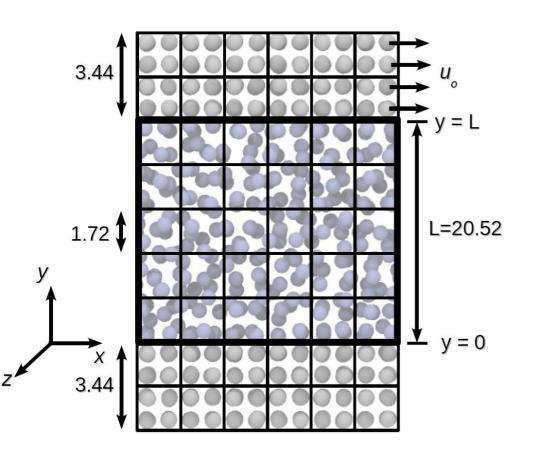
$$\frac{d}{dt}\sum_{i=1}^{N}m_i\mathbf{v}_i\vartheta_i = \sum_{i,j}^{N}f_{xij}dS_{yij}^+ - \sum_{i,j}^{N}f_{xij}dS_{yij}^-$$

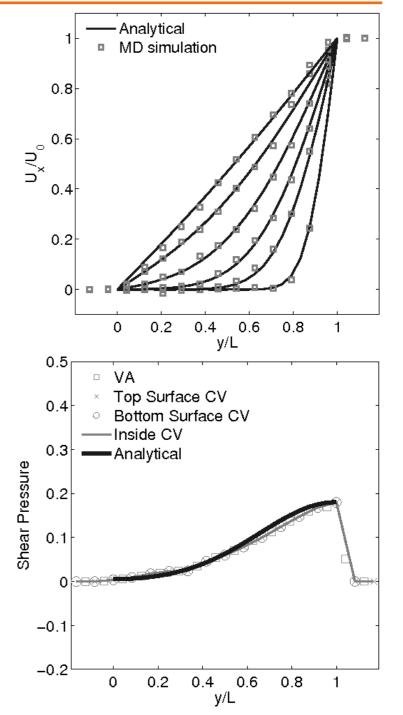
$$\frac{\partial}{\partial t} \int_{V} \rho u_{x} dV = \int_{S_{f}^{+}} \Pi_{xy} dS_{f}^{+} - \int_{S_{f}^{-}} \Pi_{xy} dS_{f}^{-}.$$



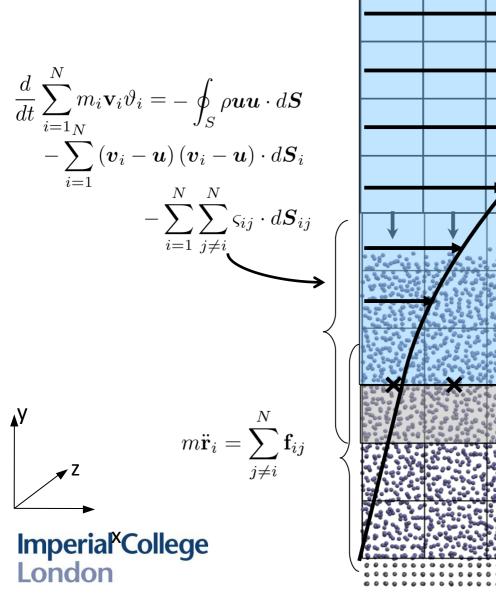
. Simulation setup

- Starting Couette flow
- · Wall thermostat: Nosé-Hoover
- Averages are computed over 1000 time steps and 8 realizations





Coupling



Molecular

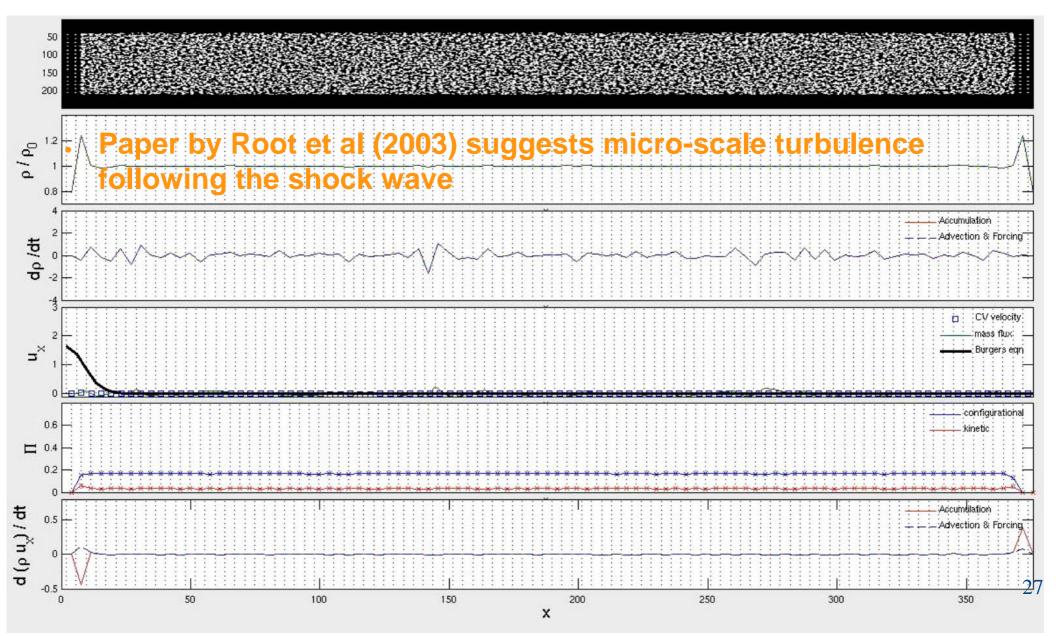
Equations

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Shockwaves

Current work on application of control volume theory

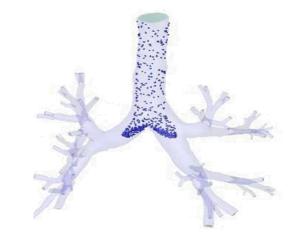
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Other Possible Applications

Particles laden continuum flows

- . Sediment transfer in rivers
- Tracer particles in flow analysis
- . Vortex particle methods
 - Discrete Lagrangian vortices which interact
- . Other discrete meso-scale methods
 - Brownian dynamics
 - Dissipative particle dynamics
 - Smooth particle hydrodynamics
- . Analysis of results from discrete experiments
 - Volumetric 3-component velocimetry



Summary

- Introduced a novel mathematical function to defines a control volume in a discrete system
 - Derived in a manner consistent with a continuum form of the control volume
 - Mathematically well defined and applicable to any discrete system
- . Reynolds' transport theorem is extended beyond the continuum
 - Allows control volume analysis to be extended to nano-scale systems
 - The resulting equations are exactly conservative in a discrete system
- . The resulting formulation has a number of applications
 - Give a consistent and intuitive form of molecular pressure showing the connection between two widely used descriptions in the literature
 - . Semi-analytical solution to problems like Couette flow
 - Facilitates a rigorous derivation of coupling strategies
 - Analysis of shockwaves and insight into molecular level turbulence.

References/Acknowledgments

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- My supervisors; Professor D.M.
 Heyes, Dr D. Dini and Dr T.A. Zaki
- Dr Nolan for his photographs

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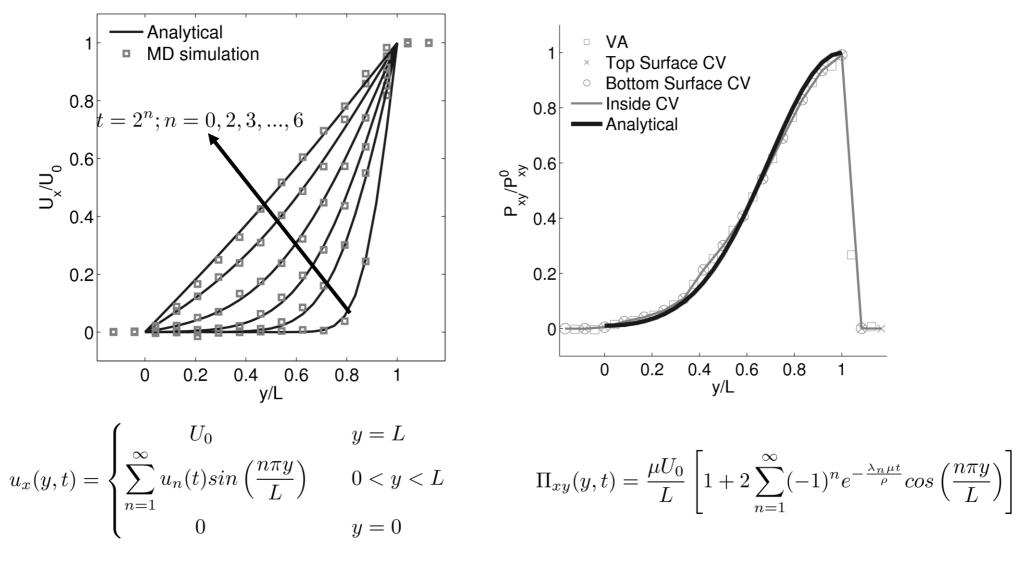
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. Thank you for listening

Any Questions?

Continuum Analytical Couette Flow



Where, $\lambda_n = \left(\frac{n\pi}{L}\right)^2$ and $u_n(t) = \frac{2U_0(-1)^n}{n\pi} \left(e^{-\frac{\lambda_n \mu t}{\rho}} - 1\right)$ **Imperial College** 31

Moving reference frame

- Why the continuum form of Reynolds' transport theorem has a partial derivative but the discrete is a full derivative
 - Eulerian mass conservation

$$\frac{d}{dt}\sum_{i=1}^{N}m_i\vartheta_i = -\sum_{i=1}^{N}m_i\mathbf{v}_i \cdot d\boldsymbol{S}_i$$

$$\vartheta_i = \vartheta_i(\boldsymbol{r}_i(t), \boldsymbol{r})$$

$$\frac{\partial}{\partial t} \int_{V} \rho dV = -\oint_{S} \rho \boldsymbol{u} \cdot d\mathbf{S}$$

Lagrangian mass conservation

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \vartheta_i = -\sum_{i=1}^{N} m_i \left(\mathbf{v}_i + \overline{\boldsymbol{u}}\right) \cdot d\boldsymbol{S}_i$$

 $\overline{\boldsymbol{u}} \cdot d\boldsymbol{S}_i = \frac{d\boldsymbol{r}}{dt} \cdot \frac{d\vartheta_i}{d\boldsymbol{r}}$

$$\vartheta_i = \vartheta_i(\boldsymbol{r}_i(t), \boldsymbol{r}(t))$$

$$\frac{d}{dt} \int_{V} \rho dV = \oint_{S} \rho \left(\boldsymbol{u} - \overline{\boldsymbol{u}} \right) \cdot d\boldsymbol{S}$$

$$\oint_{S} \rho \boldsymbol{u} \cdot d\boldsymbol{S} - \oint_{S} \rho \overline{\boldsymbol{u}} \cdot d\boldsymbol{S} = 0$$